Thermodynamic Modeling

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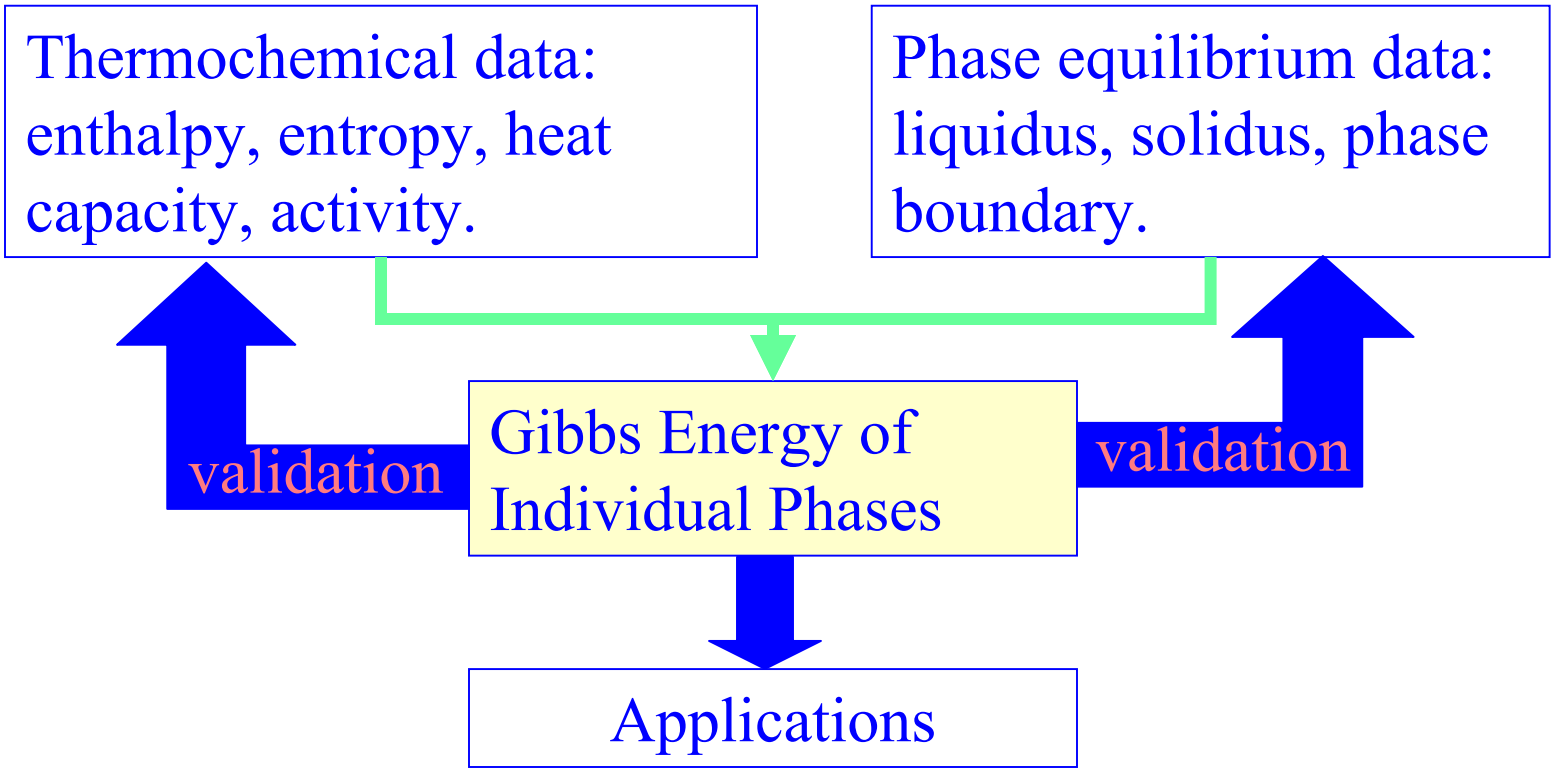
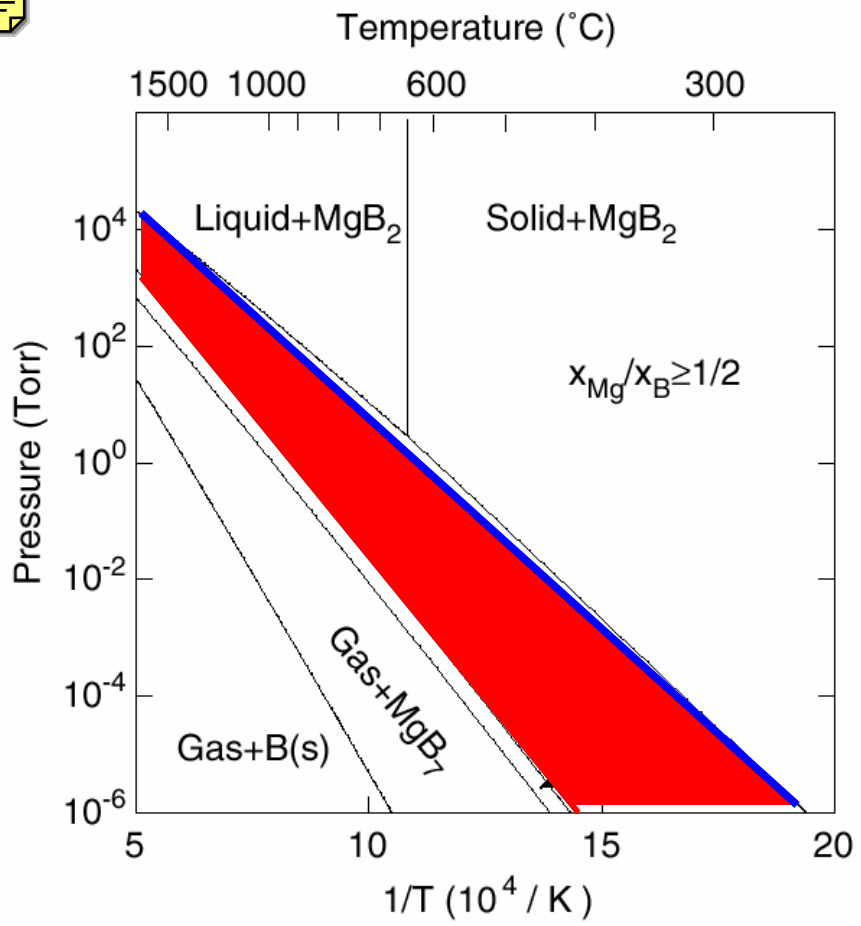


The Integration of Thermochemical and Phase Equilibrium Data is the Key.

- Two communities: Thermochemical study and phase equilibrium study, but they are two aspects of thermodynamics, one on derivatives and other on minimization. Only the combination of these two can unambiguously determine the thermodynamic property of a system.
- Gibbs energy is the free energy minimized under constant T and P, typical experimental conditions. That is why Gibbs energy is modeled instead of other free energy.
- The modeling of Gibbs energy of individual phases makes it feasible to treat multicomponent systems. This is why CALPHAD modeling has been successful.
- The modeling can be validated through new experiments and applications.

Pressure-Temperature Phase Diagram for x_{Mg}/x_B>1/2



Process window: where the thermodynamically stable phases are **Gas+MgB_2**.

— Mg partial pressure has to be high enough to keep MgB_2 phase stable

— Mg partial pressure should not be too high to avoid solid or liquid phases

Mg partial pressure *P* can be converted to Mg flux *F*:

$$F = \frac{P}{\sqrt{2\pi\, m\, k_B\, T}}$$

Phase diagram same for all Mg:B ratio above 1:2.

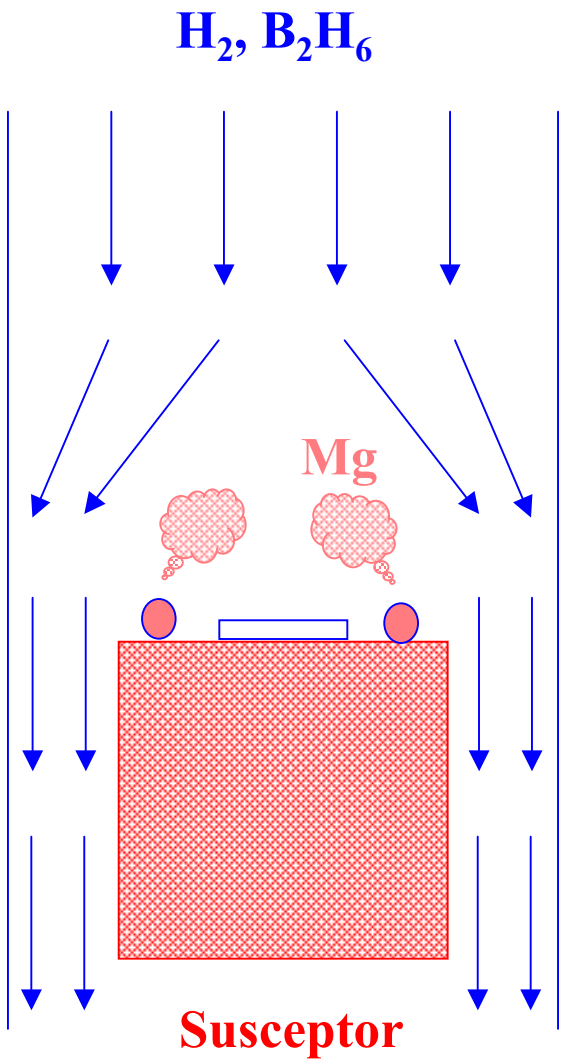
Phase Boundaries:

log (*P*) = -7561/*T* + 8.673 (Upper)

log (*P*) = -10142/*T* + 8.562 (Lower)

(Liu et al. APL 78, 3678 (2001))

Hybrid Physical-Chemical Vapor Deposition



P_{total} = 100 - 700 Torr
P_{Mg} > ?

Total flow: 1 slm
B_2H_6 mixture (1000 ppm in H_2): 25 sccm

Temperature: 730 – 760 °C

Deposition rate: 2-3 Å/sec

Provisional patent applied

The experimental setup is schematically shown.

The Mg molten droplets around the substrate provide sufficient Mg partial pressure (above the lower, red boundary in the an earlier slide), but it is also lower than the upper, blue boundary so there will be no Mg deposition on the film. This is because the Mg partial pressure at the upper boundary is only maintained very close to the Mg droplets, anywhere else, the Mg partial pressure will be lower than that.

Again, the flux B2H6 is an important processing parameter here.

Resistivity of MgB_2 film on SiC substrate